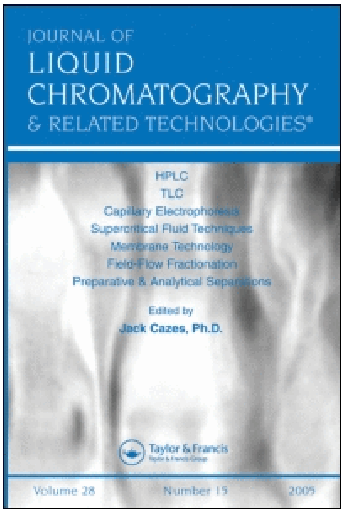

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An Example of Information Exchange Between a Liquid Chromatographic System And a Robotic Sample Preparation System

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AN EXAMPLE OF INFORMATION EXCHANGE BETWEEN A LIQUID CHROMATOGRAPHIC SYSTEM AND A ROBOTIC SAMPLE PREPARATION SYSTEM

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Analytical laboratories are looking for the "Total Solution" today. Ideally, the "Total Solution" is the automation of all steps after receiving a sample for analysis including generation of the final report. While that goal is not yet fully realized, efforts to attain it are well underway. Robotic sample preparation systems have rapidly evolved to become common tools in many analytical laboratories which use them along with standard analytical instruments such as chromatographs and spectrophotometers. Physically coupling the two types of systems can offer advantages -- the full extent of which depends upon the degree of sophistication in the communication between them. The goal of a "Total Solution" demands real-time decision-making capability based on the information associated with each sample. This information includes everything from its origin to just-completed chromatographic results as the sample travels through the lab. Hence, the level of information exchange between preparation and analysis systems will determine how fully the potential power of such a coupling is utilized.

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Interface modules, generically referred to as Module Support Boards (MSB), have been developed to facilitate the exchange of data and sophisticated control functions between Zymark laboratory automation systems and Hewlett-Packard analytical instruments such as gas and liquid chromatographs and UV/VIS spectrophotometers. Sample identification and tracking can be incorporated using barcode labels which the user generates at the location of his choice to encode sample information pertinent to him. Adding a personal computer allows algorithmic designation of preparation and instrumental method according to sample identity and/or analytical results.

Advantages of higher level communications can be seen in the following example. A sample with a barcode label encoding the information that it is the first sample originating in the Avondale facility in Lab #3 (AV/L3/1) is presented to the robotic sample preparation system for work-up and hand-off to a chromatographic system. Original sample information, preparation information, and the chromatographic method to be used are sent to the chromatographic system to direct the analytical conditions, annotate the report, and quantitate analytes. Results of the analysis are sent to the sample preparation system by the chromatographic system for simple if/then decision making to direct further sample preparation.

The example just outlined was implemented for LC analysis using an HP1090 liquid chromatographic system and a Zymark sample preparation system (Figure 1). [Similar configurations have been used for gas chromatographic systems (1).] An integrator report showing the LC results and analyte quantitation is presented in Figure 2. Note that the report incorporates information passed from the Zymate system specific to the sample and its preparation: sample identity and history, quantities of sample solution and internal standard, and robotic prep history of the sample via the rack index. The quantitative result for each analyte peak was sent to the Zymate system immediately following report generation. At that time, had the application required it, simple decisions could have been made in the Zymate system as to the next preparation operations to follow. Applications where this would be useful are those requiring confirmation and concentration bracketing.

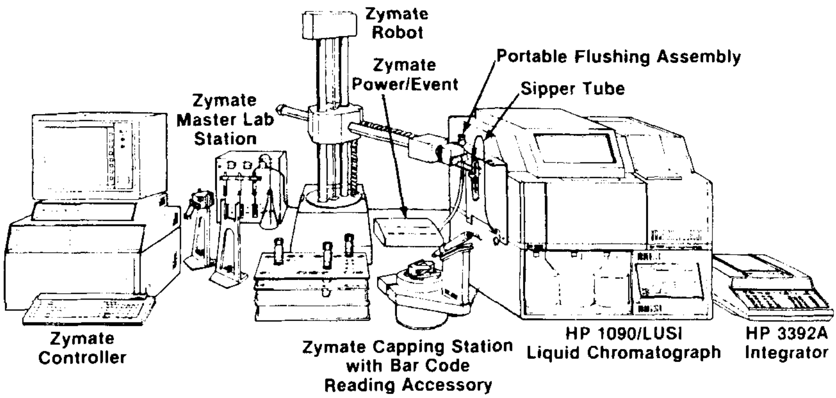

Figure 1. A Zymark automatic sample preparation system coupled to a Hewlett-Packard LC system.

HP1090 Liquid Chromatograph systems are configured from modular components (solvent delivery system, injection/sampling system, detectors, controllers and external devices)according to the requirements of the user's application. In the example shown here, the LC included a Robotic Interface Module for sample introduction from the robotic system(2), a filter photometric detector with the 7 standard filters installed, a local user communications interface (LUSI) controller with the INET communications to an HP3392A integrator, a ternary DR5 solvent deliver system, and a heated column compartment. The Zymate capping station shown in Figure 1 has been enhanced with a barcode reading assembly to read barcode labels placed about the circumference of sample vessels (Figure 3a). The information, transferred to the Zymate controller via the barcode reader MSB, is uploaded to the integrator in the chromatographic system for report annotation as shown in Figure 2. Sample identification becomes positively associated with the sample (not just a position in the preparation sequence) and that identification can be incorporated in the integrator report. Chemically resistant barcode labels can be generated by the user with a portable barcode system (Figure 3b). The information encoded by the barcode (e.g., the date, time and place of sample origination; the person who took the sample; the various preparation and analytical methods to use on the specific sample) is easily designated by the user at the time he is generating the labels. When the identification is some alphanumeric phrase chosen by the user according to his record keeping system for sample flow through the laboratory, his bookkeeping can be greatly simplified and considerably more accurate.

Major decisions in sample preparation and analytical procedures are dependent upon the information provided by the sample identity and the information contained in the results of a previous analysis of a sample. Two levels of communication based on using MSB's as the basic interface between the analytical and preparation systems have been explored.

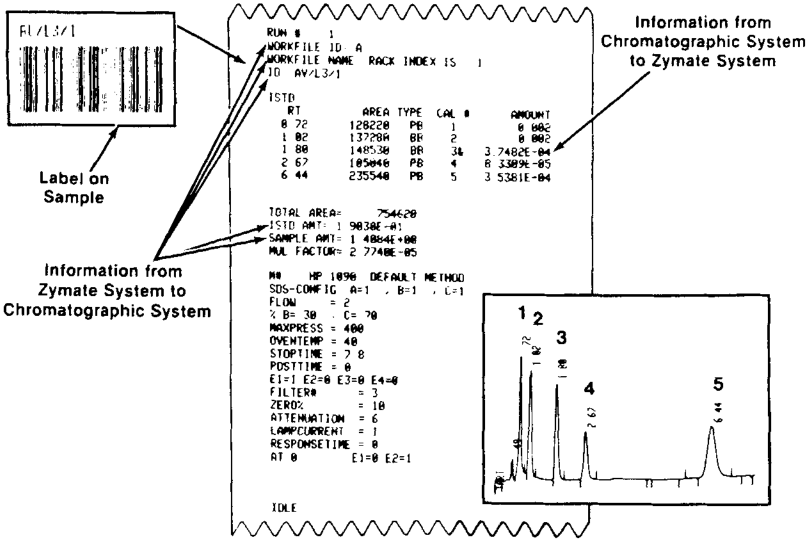

Figure 2. Chromatogram and report from an HP1090 LC showing quantitation by an internal standard, preparation information, and sample identification read from the barcode-labeled sample solution. Quantitation, under "AMOUNT", is presented as analyte weight % of original solution. An aliquot of 20 µL of sample spiked with an internal standard was injected; analyte levels ranged from tens of nanograms up. Solution components are dimethylphthalate (1), diethylphthalate (2), naphthalene as internal standard (3), biphenyl (4), and o-ter-phenyl (5) in methanol. Chromatographic conditions not noted on the figure: isocratic development; mobile phase 30/70 water/methanol; 254 nm; Hypersil ODS column, 10 cm x 4.6 mm ID, 5 µm particle diameter (HP Part No. 79916)D-554).

They differ in the degree to which the exchanged information can be used to drive the procedures (3).

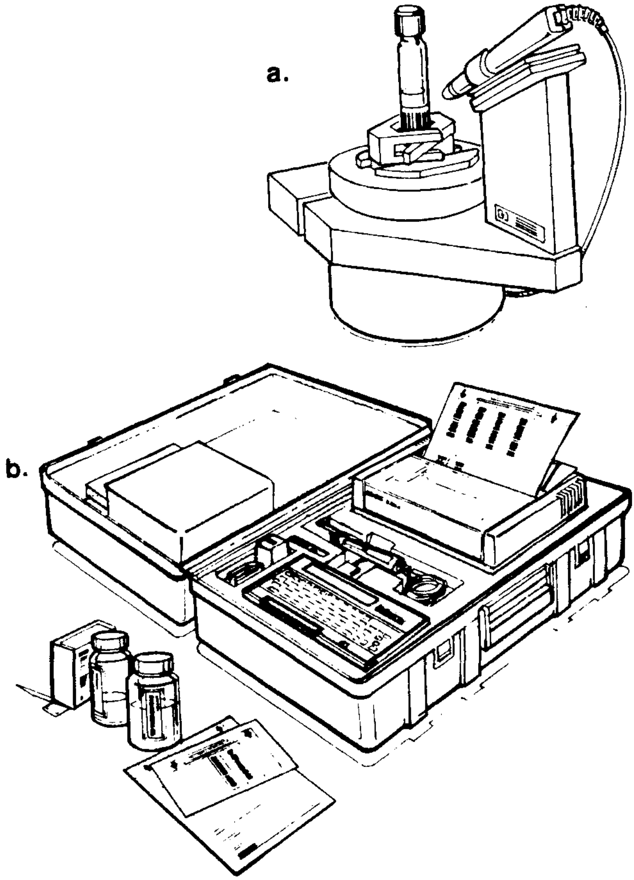

Figure 3. Barcode modules: a. Zymark (screw) capping station upgraded with a Z374 to provide barcode reading capability and b. the HP7690A protable barcode system with computer, wand, printer, manuals, and consummables packaged in a large attache carrying case.

In the first, simple if/then decision-making capability resides solely in the Zymark controller. That level is configured from a Zymark system and an analytical system and does not include an additional computer. In the second level, algorithmic control of both the sample preparation and the analytical method is gained by adding a (personal) computer, such as an HP Vectra PC. Besides the capability of making choices as to which instruments (LC, GC or both), preparation procedures and analytical methods to use, a PC in the system allows spread sheet manipulation and long-term archival storage.

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